

Diethylmalonic acid, monochloride, isopropyl ester

Inchi:	InChI=1S/C10H17ClO3/c1-5-10(6-2,8(11)12)9(13)14-7(3)4/h7H,5-6H2,1-4H3
InchiKey:	BPMFMWNXGVXGMX-UHFFFAOYSA-N
Formula:	C10H17ClO3
SMILES:	CCC(CC)(C(=O)Cl)C(=O)OC(C)C
Mol. weight [g/mol]:	220.69

Physical Properties

Property code	Value	Unit	Source
gf	-341.05	kJ/mol	Joback Method
hf	-636.88	kJ/mol	Joback Method
hfus	19.30	kJ/mol	Joback Method
hvap	56.46	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.510		Crippen Method
mcvol	173.010	ml/mol	McGowan Method
pc	2313.61	kPa	Joback Method
rinqol	1174.00		NIST Webbook
tb	592.12	K	Joback Method
tc	791.38	K	Joback Method
tf	341.89	K	Joback Method
vc	0.657	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.07	J/molxK	592.12	Joback Method
cpg	435.71	J/molxK	625.33	Joback Method
cpg	448.58	J/molxK	658.54	Joback Method
cpg	460.71	J/molxK	691.75	Joback Method
cpg	472.11	J/molxK	724.96	Joback Method
cpg	482.81	J/molxK	758.17	Joback Method
cpg	492.83	J/molxK	791.38	Joback Method
dvisc	0.0033109	Paxs	341.89	Joback Method
dvisc	0.0015851	Paxs	383.59	Joback Method

dvisc	0.0008768	Paxs	425.30	Joback Method
dvisc	0.0005391	Paxs	467.00	Joback Method
dvisc	0.0003590	Paxs	508.71	Joback Method
dvisc	0.0002543	Paxs	550.41	Joback Method
dvisc	0.0001890	Paxs	592.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370281&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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